



Uncertainty in Damage Detection, Dynamic Propagation and Just-in-Time Networks

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Final Report

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14. ABSTRACT <p>We report significant findings in three distinct areas of investigation: I. Uncertainty Quantification: Propagation and Stochastic Systems; II. Numerical Interface Methods; III. Non-smooth Variational Problems and Inverse Methods. Topics investigated include effects of different types of delays on the dynamics of stochastic systems; the performance of different methods for quantifying parameter uncertainty due to measurement error: asymptotic theory, bootstrapping, and Bayesian estimation; very general optimal design problem for the selection of best states to observe and optimal sampling times and locations (i.e., selections of what, when, and where to observe) for parameter estimation or inverse problems involving complex nonlinear partial differential equation, ordinary differential equation and/or delay differential equation systems; the identification of thermal degradation using probabilistic models in reflectance spectroscopy; optimal control based ideas (bang-bang system stimulation) for enhancing the information content and minimizing related estimated parameter uncertainty in dynamic data sets; high order compact finite difference schemes for Helmholtz equations with discontinuous wave numbers across interfaces; numerical sensitivity analysis with</p>					
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Uncertainty in Damage Detection, Dynamic Propagation and Just-in-Time Networks

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Final Technical Report

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PI: H.T. Banks Co-PI: S. Hu, K. Ito, Z. Li

H. T. Banks and S. Hu

I. Uncertainty Quantification: Propagation and Stochastic Systems

Uncertainty propagation and quantification has gained considerable research attention during recent years. In our efforts to date we consider uncertainty propagation and quantification in a continuous-time dynamical system governed by ordinary differential equations with uncertain/stochastic components. Specifically, we focused on the time evolution of probability density functions of the resulting stochastic processes, and discussed their applications in different fields with particular focus on population dynamics. In addition, we compared the difference in the stochastic processes resulting from differential equations with different types of random inputs, and discussed the connections among them.

In other efforts, we investigated the effects of different types of delays, a fixed delay and a random delay, on the dynamics of stochastic systems as well as their relationship with each other in the context of a just-in-time network model. The specific example on which we focus is a production network model with transport delays. We numerically explored the corresponding deterministic approximations for the stochastic systems with these two different types of delays. Numerical results reveal that the agreement of stochastic systems with fixed and random

delays depend upon the population size and the variance of the random delay, even when the mean value of the random delay is chosen the same as the value of the fixed delay. When the variance of the random delay is sufficiently small, the histograms of state solutions to the stochastic system with a random delay are similar to those of the stochastic model with a fixed delay regardless of the population size. We also compared the stochastic system with a Gamma distributed random delay to the stochastic system constructed based on the Kurtz's limit theorem from a system of deterministic delay differential equations with a Gamma distributed delay. We found that with the same population size the histogram plots for the solution to the second system appear more dispersed than the corresponding ones obtained for the first case. In addition, we found that there is more agreement between the histograms of these two stochastic systems as the variance of the Gamma distributed random delay decreases.

In further efforts on uncertainty quantification, we compared the performance of three methods for quantifying parameter uncertainty due to measurement error: asymptotic theory, bootstrapping, and Bayesian estimation. We used an existing model for one-dimensional wave propagation in a viscoelastic medium, as well as corresponding data from lab experiments using a homogeneous, tissue-mimicking gel phantom. The results from the three algorithms quantify complex correlations between our model parameters, which is best seen using the more computationally expensive bootstrapping or Bayesian methods. We fixed the parameter causing the most complex correlation, and then obtained results from all three methods which demonstrate very similar quantification of the parameter uncertainty. Concerns regarding computational time and algorithm complexity are also considered.

In year 2 of our grant period, we continued our efforts on methodology development combining uncertainty quantification in statistical and applied mathematical problems. In one effort we formulate a very general optimal design problem for the selection of best states to observe and optimal sampling times and locations (i.e., selections of what, when, and where to observe) for parameter estimation or inverse problems involving complex nonlinear partial differential equation, ordinary differential equation and/or delay differential equation systems. A theoretical framework based on the Fisher Information Matrix along with a detailed iterative algorithm for implementation of the resulting methodology have been developed and the algorithm's successful use on several examples of wide

interest has been demonstrated. Among these is an application to electromagnetic interrogation problems for brain scans.

We have considered an electromagnetic interrogation problem, specifically one arising in an electroencephalography (EEG) problem, of finding optimal number and locations for sensors for source identification in a 3D unit sphere from data on its boundary. In this effort we compared the use of the classical D-optimal criterion for observation points as opposed to that for a uniform observation mesh. We considered location and best number of sensors and reported results based on statistical uncertainty analysis of the resulting estimated parameters.

In a second major thrust, we investigated the properties of a complex nonmagnetic material through the reflectance, where the permittivity is described by a mechanism model in which an unknown probability measure is placed on the model parameters such as relaxation constants and/or reflection wave numbers. Specifically, we considered whether or not this unknown probability measure can be determined from the reflectance and/or the derivatives of the reflectance, and we also investigated the effect of measurement noise on the estimation. For relaxation constants, the numerical results demonstrate that if only the reflectance can be observed, then the distribution form cannot be recovered even in the case where the measurement noise level is small. However, if both the reflectance and the derivative of the reflectance can be observed, then the estimated distribution is reasonably close to the true one even in the case where the measurement noise level is relatively high. In the case of distributions on wave numbers, we are able to demonstrate that reflectance data alone is sufficient to develop efficient algorithms. We have demonstrated the feasibility of our proposed methods by numerical results obtained for both simulated data and experimental data for inorganic glass.

Some of these investigations involve the identification of thermal degradation using probabilistic models in reflectance spectroscopy and were carried in collaboration with scientists at AFRL (Materials State Awareness & Supportability Branch, Air Force Research Lab, WPAFB 45433, USA) lead by Amanda K. Criner and Adam T. Cooney. Different probabilistic models of molecular vibration modes are considered to model the reflectance spectra of chemical species through the dielectric constant. Probability measure estimators in parametric and nonparametric models are being considered. Analyses of ceramic matrix composite samples that have been heat treated for different amounts of times are

being studied. These results will be compared with the analysis of vitreous silica using nonparametric models.

The efforts involve computational methods and their convergence results that have been developed by our group in the past two decades for nonparametric estimation of probability measures from aggregate data using least-squares or generalized least methods under the Prohorov Metric Framework. New results are presented on the consistency of the probability measure estimator, the bias due to the approximation and the pointwise asymptotic normality of the approximated probability measure estimator.

In the final year of our efforts on this grant we have emphasized model-based optimal design methodology (which variables to observe, when, where and how often measurements should be taken, etc.). As part of this thrust we have developed techniques (using Fisher Information Matrix-based efforts and model comparison ideas) to determine the type and amount of useful information content in given data sets. This has led to optimal control based ideas (bang-bang system stimulation) for enhancing the information content and minimizing related estimated parameter uncertainty in various types of dynamic data sets.

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Zhilin Li

II. Numerical Interface Methods

Summary of efforts and findings:

- The PI spent significant amount of time to carry out the research and other activities related to the proposal including
- Literature search, reading, and review
- Derive mathematical models, new numerical methods, and study the convergence of the proposed new method
- Intensive code writing to implement, validate the new methods and applied to various applications
- Regular study seminars and weekly meetings with graduate students
- Attended related conferences/meeting both in domestic and international
- Presented talks at a number of international conferences/workshops
- Organized related international conferences/workshops
- Visit other universities and institutions to exchange ideas and carry out research collaborations
- Research collaborations: UC-Irvine, Purdue University

Findings:

- We have set up the framework for augmented IIM for Navier-Stokes equations with interfaces or on irregular domains
- We developed high order compact finite difference schemes for Helmholtz equations with discontinuous wave numbers across interfaces.
- We carried out numerical sensitivity analysis with respect to the Reynolds number for the flow past obstacle problem. Such analysis enables us to predict the critical Reynolds number numerically. Various numerical experiments show such a prediction is reliable.
- In collaboration with researchers at UCI, we have provided efficient, 3D fast Poisson solver for bio-molecular simulations.
- We have developed adaptive Cartesian method for Immersed Boundary (IB) and Immersed Interface Method (IIM) for elliptic interface problems and for two phase flows with moving interfaces.

Publications:

(a) Papers published in refereed journals during this report period (title, co-authors, journal, volume number, date, page numbers).

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((b) Papers accepted by refereed journals during this report period and awaiting publication (title, co-authors, journal, number of pages).

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- Z. Li, Q. Cai, H. Zhao, R. Luo, A semi-implicit augmented IIM for Navier-Stokes equations with open, traction, or free boundary conditions, JCP, in press.

(c) Papers submitted to refereed journals during this report period and currently being refereed (title, co-authors, journal, number of pages).

- Z. Li, H. Mikayelyan, Fine numerical analysis of the crack-tip position for a Mumford-Shah minimizer, Free Boundary Problems.
- J. Ruiz and Z. Li, The Immersed Interface Method for axis-symmetric problems and application to the Hele-Shaw flow, Applied Mathematics and Computation
- Z. Li, J. Xia, Effective and efficient matrix-free preconditioner for augmented immersed interface methods, submitted to JCP.
- Ji, H. F., Chen, J. R., & Li, Z. L. A New Augmented Immersed Finite Element Method Without Using SVD Interpolations, submitted to Numerical Algorithm

K. Ito

III. Non-smooth Variational Problems and Inverse Methods

We have developed and analyzed efficient numerical methods for non-smooth variational problems including optimization problems that have important applications in structural design and control problems, image and compress sensing and inverse problems. The Lagrange multiplier theory has been developed for the sparsity optimization with ℓ_0 regularization [6], where ℓ_0 is the cardinality of nonzero elements of vector unknowns. The ℓ_0 regularization method is a very effective formulation that results in a sharp sparse solution. But, since it is non differentiable and non convex functional and thus it is non trivial to analyze the corresponding optimization problem and develop optimization algorithms.

Based on our theory a semi-smooth Newton method in the form of Primal-Dual active set method is developed. It is a very efficient and effective method. The method has been tested for the de-convolution problems and we demonstrated its applicability and feasibility. We also analyze the global convergence of the algorithm under certain strict complementarity condition. The extension to optimization problems with $L_0(D)$ metric for the material design and control problems has been investigated [7].

A weak form of fluid-structure interaction was developed. We use a shape derivative of the deformation energy to derive the weak form. The level set formulation of fluid structure interaction as well as discrete deformation energy formulation are discussed and analyzed. Based on the formulation we have energy conservation and establish existence of weak solutions. We also present numerical tests for demonstrating our formulation, especially for a fluid-structure interaction that models a biomedical micro-electro-mechanical system.

A new staggered-grid based central finite difference scheme is developed for Stokes and Navier-Stokes equations and Maxwell equations. The staggered grid is only for the pressure node, i.e., the pressure grid is the center of the square cell and the velocities are at the regular node. The advantage of the proposed method compared to the Marker & Cell method is that it is very straightforward to treat the boundary conditions for the velocity field, the transport equation, the fluid structure interaction and the multiphase flow. We develop the difference scheme for the convective term that preserves the dissipation property for the incompressible Navier-Stokes equation. We have also developed and analyzed the implicit and explicit time integration method for the incompressible Navier-Stokes equation. The method has been tested for the driven cavity flow and the fluid-structure interaction.

We have also continued our effort for developing and testing the probing method for inverse medium problems. Specifically, it has been investigated for the electric impedance tomography (EIT) [11] and the diffusive optical tomography (DOT) [13]. Our method for (EIT) and (DOT) creates images of the electrical conductivity and the absorption of an inhomogeneous medium. We use the dipole test function to generate the likelihood distribution (probing index) of the inhomogeneity of the medium. We have tested and analyzed the probing method

for two and three dimensional cases where the effectiveness of a probing index is demonstrated.

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1.

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Program Manager**The AFOSR Program Manager currently assigned to the award**

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Reporting Period Start Date

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Abstract

We report significant findings in three distinct areas of investigation: I. Uncertainty Quantification: Propagation and Stochastic Systems; II. Numerical Interface Methods; III. Non-smooth Variational Problems and Inverse Methods. Topics investigated include effects of different types of delays on the dynamics of stochastic systems; the performance of different methods for quantifying parameter uncertainty due to measurement error: asymptotic theory, bootstrapping, and Bayesian estimation; very general optimal design problem for the selection of best states to observe and optimal sampling times and locations (i.e., selections of what, when, and where to observe) for parameter estimation or inverse problems involving complex nonlinear partial differential equation, ordinary differential equation and/or delay differential equation systems; the identification of thermal degradation using probabilistic models in reflectance spectroscopy; optimal control based ideas (bang-bang system stimulation) for enhancing the information content and minimizing related estimated parameter uncertainty in dynamic data sets; high order compact finite difference schemes for Helmholtz equations with discontinuous wave numbers across interfaces; numerical sensitivity analysis with respect to the Reynolds number for the flow past obstacle problems; efficient, 3D fast Poisson solver for bio-molecular simulations; adaptive Cartesian method for Immersed Boundary (IB) and Immersed Interface Method (IIM) for elliptic interface problems and for two phase flows with moving interfaces; efficient numerical methods for non-smooth variational problems; staggered-grid

based central finite difference scheme is developed for Stokes and Navier-Stokes equations and Maxwell equations; probing methods for inverse medium problems, including electric impedance tomography and the diffusive optical tomography; use of dipole test functions to generate the likelihood distribution (probing index) of the inhomogeneity of the medium.

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Reporting Period

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Technical Summary

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